GLOBAL SHAPE DEFINITION METHOD FOR SCATTEROMETRY

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Priority Claim

5   The present application claims priority to U.S. Provisional Patent Application Serial No. 60/463791, filed April 18, 2003, the disclosure of which is incorporated in this document by reference.

Technical Field

The subject invention relates generally to optical methods for inspecting and 10   analyzing semiconductor wafers and other samples. In particular, the subject invention relates to methods for modeling samples for scatterometry and other applications.

Background of the Invention

As semiconductor geometries continue to shrink, manufacturers have increasingly turned to optical techniques to perform non-destructive inspection and analysis of 15   semiconductor wafers. Optical techniques typically apply an incident field (often referred to as a probe beam) to a sample and then detect and analyze the reflected energy. This type of inspection and analysis is known as optical metrology and is performed using a range of optical techniques. Scatterometry is a specific type of optical metrology that is used when the structural geometry of a sample creates diffraction (optical scattering) of 20   the incoming probe beam. Scatterometry systems analyze diffraction to deduce details of the structures that cause the diffraction to occur.

Various optical techniques have been used to perform optical scatterometry. These include broadband spectroscopy (U.S. Patent Nos. 5,607,800; 5,867,276 and 5,963,329), spectral ellipsometry (U.S. Patent No. 5,739,909) single-wavelength optical 25   scattering (U.S. Patent No. 5,889,593), and spectral and single-wavelength beam profile reflectance and beam profile ellipsometry (U.S. Patent No. 6,429,943). In addition it may be possible to employ single-wavelength laser BPR or BPE to obtain critical dimension (CD) measurements on isolated lines or isolated vias and mesas. The above cited patents and patent applications, along with PCT Application WO03/009063, US Application 30   2002/0158193, US Application 2003/0147086, US Application 2001/0051856 Al, PCT

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Application WO 01/97280, U.S. Patent No. 6,483,580, PCT Application WO 02/27288 and PCT Application WO 03/054475 are all incorporated herein by reference.

As shown in Figure 1, a typical scatterometry system includes an illumination source that creates a mono or polychromatic probe beam. The probe beam is preferably

5   focused by one or more optical components (lenses in this case) to create an illumination spot on the surface of the sample under test. A second series of optical components (lenses for this example) transports the diffracted probe beam to a detector. The detector captures the diffracted energy and produces corresponding output signals. A processor analyzes the signals generated by the detector using a database.

10   Scatterometry systems (like the one shown in Figure 1) may be used to analyze a wide range of samples. A typical example, shown in Figure 2, includes a scattering structure formed on a substrate. For this particular example, the scattering structure is a grating composed of a series of individual lines. In general, the scattering structure may be periodic (as in the case of Figure 2) or isolated. Isolated structures include, for

15   example individual lines or individual vias. The scattering structure of Figure 2 is uniform (i.e., exhibits translational symmetry) along the Y axis. For this reason, the scattering structure is considered to be two-dimensional. Three dimensional scattering structures are also possible both in isolation (e.g., single via) or periodically (e.g., pattern of vias). The scatting structure is covered by an incident medium that is typically air but

20   may be vacuum, gas, liquid, or solid (such as an overlaying layer or layers). One or more layers may be positioned between the scattering structure and the substrate. In most cases, the probe beam intersects the scattering structure at a normal angle (i.e., perpendicular to the lines that from the scattering structure). Conical scattering, where the probe beam intersects the scattering structure at a non-normal angle is also possible.

25   In most cases, a modeling process is used to translate the empirical measurements obtained during scatterometry into physical measurements such as line widths. For this process, a software model is used to represent the expected structure and composition of the sample. The software model is parameterized, allowing characteristics such as line widths and line profiles to be changed. Maxwell's equations are used to predict the

30   diffraction that the modeled structure would impart to the probe beam of the scatterometer. A set of these predicted measurements are generated using variations to

the parameters of the model. This process is repeated until the predicted measurements match the empirical measurements to a desired goodness of fit. At that point, the modeled structure and its associated parameters are assumed to match the sample.

5   To be accurate, the model used during the modeling process must reflect the structure and composition of the sample. For the example of Figure 2, this can be relatively straight-forward. The lines of the scattering structure in that example are rectangular in cross-section, allowing each line to be modeled using a small number of parameters (typically, line height and line width). Each line is further simplified by being composed of a single material and being geometrically invariant along the Y-axis. In

10   practice, this relative simplicity is not always typical of samples. Figure 3 shows, for example a sample that includes lines having rounded edges and sloping sidewalls. Adding additional complexity, the lines in the scattering structure of Figure 3 are composed of multiple layers, each of which may have different dielectric properties.

       Complex samples, such as the sample shown in Figure 3 require correspondingly

15   complex modeling techniques. For one of these techniques, a Riemannian approach is used to model geometric shapes (such as the lines) as stacks of slabs. For example, the line profile of Figure 4A may be modeled using the stack of slabs shown in Figure 4B. The height and width of each slab is chosen so that the stack of slabs approximates the shape being modeled. Portions of the shape that change rapidly (such as the foot or top of

20   the line profile of Figure 4A) can be accurately modeled by increasing the number of slabs while decreasing their thickness (not shown). Shape portions that are relatively constant may be modeled using fewer, thicker slabs. Models constructed using this technique require two parameters for each slab (height, width) or a total of 2N parameters for N slab models.

25   The slab-based technique necessarily introduces a degree of roughness into the resulting model. This roughness gives the model edges a staircase-like appearance attributable to the rectangular cross-section of the individual slabs. This side-effect can be reduced by using slabs that have a trapezoidal cross-sections or quadrilateral cross-sections. The use of trapezoid slabs is shown in Figure 4C. The overall effect is a

30   reduction in stair-stepping at the cost of additional parameters. For trapezoidal cross-sections, three parameters are required for each slab (height, width and one interior

angle). Quadrilateral cross-sections require four parameters (height, width and two interior angles).

Quadrilaterals or trapezoids are an effective method for increasing the accuracy of the modeling process. At the same time, the increased number of parameters adds further complexity to an already arduous computational process. As a result, there are continuing efforts to find modeling methods that provide high accuracy while limiting the number of required parameters. This is the goal of the method described, for example in US Patent 5,963,329 (incorporated in this document by reference). For this method, the familiar slab-based approach is used to model lines and other geometric shapes. In this case, however, the slabs are subdivided into one or more sub-profiles. Each sub-profile has a reference edge and a reference height. The width of each slab in a sub-profile is defined using an offset (which may be positive or negative) from the reference edge. The height of each slab in a sub-profile is defined as a multiple of the reference height. Each sub-profile also has two scaling factors, one for height and a second for width. Changing the height scaling factor increases or decreases the height of all of the slabs in a sub-profile making the sub-profile taller or shorter. Changing the width scaling factor spreads the sub-profile—slabs that are narrower than the reference edge become narrower still, slabs that are wider than the reference edge become even wider. By controlling the scaling factors for each sub-profile, the overall profile of the line can be varied to produce a range of differing shapes.

The use of sub-profiles and associated scaling factors decreases the number of parameters that are required to define a particular shape. Unfortunately, the use of rectangular slabs suffers from the staircase limitations already described. It is also true that the use of scaling factors is only beneficial when computational results can be re-used as the scaling factors are changed. For cases where this is not possible, the use of scaling factors is computationally similar to more traditional methods for defining slab heights and widths.

For these reasons and others, a need exists for scatterometry techniques that avoid the limitations of traditional modeling methods. This need is particularly apparent for high density semiconductor wafers where feature sizes are small.

Summary of the Invention

The present invention provides a global shape definition method for modeling samples. For this method, a control-point based approach is used to define the geometric shapes within samples. As an example, consider the case of a sample that includes one or
5   more lines. The profile (i.e., the cross-sectional outline) of a representative line is defined using a set of control points. Each control point influences the shape of the line profile. For some cases, this means that control points define shapes in a connect-the-dots fashion. For other cases, a more complex mathematical function, such as Bezier or Spline curve fitting, is used to translate a set of control points into a corresponding shape. It
10 should be noted that the control points are preferably only used to define shapes. Layers within a shape can be modeled independently.

The present invention also provides an interactive environment for building and evaluating scatterometry models based on the global shape definition method. The interactive environment allows a user to specify multilayer scatterometry models. The
15 user can add shape profiles by adding groups of control points. Once a model has been defined, the interactive environment may be used to calculate its optical response. The user may then compare the calculated optical response with an empirically generated optical response to visually assess goodness of fit. By modifying control points (by moving, adding or deleting) and changing layer properties, the user may interactively
20 arrive at an accurate model for the sample.

Brief Description of the Drawings

Figure 1 shows a prior art optical metrology system.

Figure 2 is a diagram of an idealized prior art sample.

Figure 3 is a diagram of a second idealized prior art sample.

5   Figure 4A is a diagram showing the line profile used in the sample of Figure 3.

Figure 4B is a diagram showing a model for the line profile of Figure 4A where the model is constructed using a prior art slab-based technique.

Figure 4C is a diagram showing a model for the line profile of Figure 4A where the model is constructed using a prior art trapezoidal technique.

10   Figure 5A through 5X show various samples modeled using a shape definition method as provided by an embodiment of the present invention.

Figure 6 is a diagram showing the visual design environment as provided by an embodiment of the present invention.

Figure 7 is a diagram showing the spectral display component of the visual design

15   environment of Figure 6.

Figure 8 is a diagram showing the film structure component of the visual design environment of Figure 6.

Figure 9 is a diagram showing the layer property component of the visual design environment of Figure 6.

20   Figure 10 is a diagram showing the global parameters component of the visual design environment of Figure 6.

Figure 11 is a diagram showing the additional parameters component of the visual design environment of Figure 6.

Figures 12A though 12C show equally spaced, adaptive and sigmoid methods for

25   model slicing as provided by an embodiment of the present invention.

Figure 13 is a diagram showing the interactive shape modeling component of the visual design environment of Figure 6.

Figures 14A and 14B show the film structure component and the layer property component during development of a hypothetical model.

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Figures 15A though 15C show the interactive shape modeling component and the layer property component during development of a hypothetical model.

Figures 16A though 16E show various components of the visual design environment during development of a hypothetical model.

Detailed Description of the Preferred Embodiments

The present invention provides a global shape definition method for modeling samples. For typical applications, the sample to be modeled is a semiconductor wafer of the type generally shown in Figures 2 and 3 and includes a scattering structure formed on one or more underlying layers. The lowermost of the underlying layers is commonly referred to as a substrate. The scatting structure is covered by an incident medium that is typically air but may be vacuum, gas, liquid, or solid (such as an overlaying layer or layers). In the most typical case, the scattering structure is a grating consisting of a periodic series of lines. By appropriate generalizations, other isolated or periodic features may also be modeled.

For the global shape definition method, a control-point based approach is used to define the profiles (i.e., the cross-sectional outlines) of geometric shapes within the sample. Figure 5A shows a sample 500 modeled using this approach. For this particular example, sample 500 includes three layers: an upper layer 502a, an intermediate layer 502b and a substrate 502c. Each of these layers will typically (but not necessarily) be formed using a different material type.

Sample 500 also includes a line profile 504. Line profile 504 has a height (i.e., Z dimension) and a width (i.e., X dimension) and is assumed to be invariant in the Y direction. In this example, line profile 504 includes only upper layer 502a. As will be described in more detail, this is representative and line profile 504 may include any number of layers. Line profile 504 is considered to repeat at periodic intervals in the +X and –X directions. As will be discussed later, the present invention includes controls that allow the nature of this repetition to be defined.

At a minimum two control points (Z_0 and X_0) are used to control the shape of line profile 504. The specific location of each control point may be varied to produce a range of different shapes. However, the location of each fundamental control point is also constrained according to the following rules:

$$Z_0\left(x_0, z_0\right) \quad x_0 \equiv 0$$
$$z_0 \geq 0$$

$$X_0\left(x_0, z_0\right) \quad x_0 \geq 0$$
$$z_0 = h$$

where h is the height of line profile 504. In other words, Z_0 is free to move in the Z direction and X_0 is free to move in the X direction (as long as their respective Z and X

5   values do not take on negative values). Thus, for this example, Z_0 defines line height and X_0 defines line width. In general, for the modeling method, each layer included in a line profile has at least two control points—one for height, and one or more for width. Each layer not included in a line profile has a single control point for height. Control points that define height are designated using the letter Z while those defining width are

10   designated using the letter X.

To increase the complexity of line profile 504, additional control points may be added. As shown in Figure 5B, the first additional control point (X_1) is added at the base of line profile 504. Like control point X_0, control point X_1 can only moved in the X direction. Its Z coordinate is fixed:

$$X_1\left(x_1, z_1\right) \quad x_1 \geq 0$$
15
$$z_1 \equiv 0$$

Figure 5C shows the resulting changes to sample 500 when the position of X_1 is moved to narrow the base of line profile 504. At this point, it should be clear that the control points actually define half of line profile 504. Changes to the location of any control point is mirrored onto the opposite side of line profile 504. This explains why

20   moving control point X_1 narrows the based of line profile 504 on both sides—not just the side where control point X_1 is located. In general, this use of symmetry is useful because it allows the number of control points to be minimized. Alternately, separate width varying control points may be used. This is especially useful when asymmetric line profiles are modeled.

25   Figure 5D shows sample 500 after two more control points have been added to line profile 504. The new control points (X_2 and X_3) are spaced evenly along the right edge of line profile 504. Each controls width and not height. Figure 5E shows the effect of moving control points (X_0 and X_1) while leaving the new control points (X_2 and X_3)

fixed. As shown, line profile 504 is now narrowed at the top and widened at the base. Control points (X_2 and X_3) ensure that an intermediate portion between the top and base of line profile 504 remains vertical.

Figure 5F shows an example where intermediate layer 502b has been added to line profile 504. Line profile 504 now has four control points (as mentioned previously, each layer in a line profile includes a control point for height and at least one control point for width). In this case, control points Z_0 and X_0 control the height and width of the portion of upper layer 502a that is included in line profile 504. Control points Z_1 and X_1 control the height and width of the portion of intermediate layer 502b that is included in line profile 504. Figure 5G continues this particular example by showing the result of moving the X_1 control point. As may be appreciated, the portions of line profile 504 that corresponds to intermediate layer 502b is now wider than the portion that corresponds to upper layer 502a. Figure 5H and 5I show the result of adding (and then moving) an additional control point X_2. In this case X_2 has been added to the base of the portion of line profile 504 that corresponds to upper layer 502a. Movement of X_2 has narrowed that the base of that portion creating a sloping sidewall analogous to the example shown in Figures 5B and 5C.

Spacers

As shown in Figure 5J, the modeling method may also be used to define layers that cover the sidewall of line profile 504. This type of structure, known as a "spacer" is unusual in the sense that it resembles a type of coating more than a traditional layer. The modeling method allows each line profile to have one or more associated spacers. Each is defined by its thickness and material type. Once defined, spacers follow the shape of the underlying line profile 504. This is shown, for example, in Figure 5K.

Trench Fills

Trench fills are another type of structure that can be added using the modeling method. One or more trench fills may be added to each model, each specified by its thickness and material type. Figure 5L shows a model 500 that includes a single trench fill as well as a spacer. Figure 5M shows the same model after movement of two control points.

Global Shape Definition Option

In each of the preceding examples, control points are allocated on a per-layer basis. Each layer included in a line profile has a single control point that defines its height. Each layer also has one or more control points that define its width. Where more than one width defining control points is used, the result is typically a sidewall whose width varies in some way as a function of height (see examples 5C, 5E and 5I). It should be noted that the position of the width defining control points in one layer has no bearing on the size or shape of adjacent layers. The influence of control points is strictly local to the layers in which they are included. As an alternative, the modeling method may be configured to use global shape definition. To describe the global shape definition option, Figure 5N and 5O show two instances of a sample 500. In 5N, the previously described non-global method is used. Figure 5O shows a similar sample constructed using the global shape definition option. In both Figures, line profile 504 includes two layers (upper layer 502a and intermediate layer 502b). In Figure 5N (constructed with the local option) upper layer 502a includes control points Z_0, X_0, while lower layer 502b includes control points Z_1 and X_1. In Figure 5O (constructed with the local option) the height varying control points (Z_0 and Z_1) are unchanged. The two width varying control points (X_0 and X_1) have been replaced by a single control point X_0 that controls the width of both layers. Figure 5P shows the globally represented sample 500 after a movement of control point X_0. As may be appreciated, movement of the single control point has altered all portions of line profile 508 and is not limited to any layer 502.

Figure 5Q continues this example by showing a globally constructed sample 500 that includes two layers 502 within the line profile 508. A total of four control points (X_0, X_1, X_2 and X_3) define the sidewall of line profile 508. It should be noted that the control points (X_0, X_1, X_2 and X_3) are spaced uniformly along line profile 508. Their positions are independent of the layers 502a and 502b included in line profile 508. Figure 5R shows the same sample after the movement of control points X_2 and X_3. The result is a deformation of the sidewall of line profile 508 that is unrelated to the included layers 502a and 502b.

Upper layer 502a has a total of five control points (Z_0, X_0, X_1, X_2 and X_3). Intermediate layer 502b has two control points (Z_1 and X_4). In Figure 5N, the control

points X_0, X_1, X_2 and X_3 are evenly distributed over the sidewall of upper layer 502a. This follows because they directly control the shape of the portion of line profile 504 that corresponds to upper layer 502a. In Figure 5O, the control points X_0, X_1, X_2 and X_3 are evenly distributed over the sidewall of both upper layer 502a and intermediate layer

5   502b. This follows because they control the entire sidewall of line profile 504.

The global option is notable, not just because the effect is different, but also because global shape definition effectively decouples profile definition from layer properties. When the global option is used, each layer requires only a single control point to define layer height. The remaining control points are shared between layers.

10   Depending on the layers used and the profile shape, this can result in a further reduction in control points.

Local Distortion Option

When the global shape definition option is active, each control point contributes to the overall shape of the line profile. To add flexibility, the modeling method allows

15   local distortions to be added to create localized perturbations. To illustrate, Figure 5S shows a model of a sample 500 that includes a local distortion. Sample 500 includes a total of four layers: an upper layer 502a, two intermediate layers 502b and 502c and a substrate 502d. Each of the non-substrate layers is included within the line profile of sample 500. The shape of that profile is controlled by width-varying control points X_0

20   and X_1 and height varying control points Z_0, Z_1 and Z_2.

Intermediate layer 502b is configured to include a local distortion. The same layer is also configured to "snap to top." This ensures that the uppermost point in the sidewall of intermediate layer 502b has the same width as the lowermost point in the sidewall of upper layer 502a. In other words, a smooth transition is enforced between layers 502a and

25   502b. The smooth transition means that there is no need for a control point at the top of intermediate layer 502b (typically, all layers include a control point at that position (see preceding examples)). As a result, the control point X_2 for intermediate layer 502b is relocated to a point intermediate between the top and bottom of intermediate layer 502b.

Figure 5T shows the effect of moving the control point X_2. The result is a

30   distortion that is limited to the portion of line profile 504 that is included within the top and bottom of intermediate layer 502b. Subsequent movements of other control points

will change the global shape of line profile 504 but the local distortion will be maintained.

Modeling Non-Uniformities for Line Tops

For the models described above, each layer has at most one height varying control

5   point Z. To support more complex models, it is useful (in some cases) to add additional height varying control points within a single layer. As an example, consider the line profile 508 shown in Figure 5U. In this case, line profile 508 has the width varying control point X_0 along with height varying control point Z_0 originally described for Figure 5A. Line profile 508 also has an additional height varying control point Z_1 not

10   included in the example of Figure 5A. The additional height varying control point Z_1 is (at the time of initial definition) coincident with control point Z_0. As shown in Figure 5V, moving the control point Z_1 has the effect of creating a depression in the top line profile 508. The overall height of line profile 508 is still controlled by control point Z_0. This is a simple example of a line profile that can not be modeling using the previously described

15   single height varying control point per layer.

A more complex example is present in Figures 5W and 5X. As shown in Figure 5W, two additional height varying control points (Z_1 and Z_2) have been added to the line profile 508 originally show in Figure 5A. After a hypothetical movement of the additional control points, the line profile 508 of Figure 5X is obtained. Once again, the

20   overall height of line profile 508 is still controlled by control point Z_0.

The use of additional height varying control points provides a simple mechanism for extending the flexible sidewall modeling techniques to line tops. Using this technique, line tops may be arbitrarily shaped to represent a range of empirically encountered line profiles.

25   **Spline Implementation**

In general, it should be noted that a wide range of techniques may be used to translate the position of control points into corresponding curves. Of these, the simplest is to connect individual control points using straight line segments (i.e., a connect-the-dots approach). For the purposes of the present invention, it is more useful to use an approach

30   that allows control points to describe arbitrary curves. Bezier and Spline functions are two examples of techniques of this type. For the specific implementation being described,

a shape preserving B-spline curve is used to form the line profile 504. In cases where a small number of control points are used (e.g., Figure 5A, 5B and 5C) the result is that the individual control points are connected by straight lines (or at least appear to be connected by straight lines). For more complex structures, where more control points are

5   used (e.g., Figures 5M and 5R) the individual control points appear to be connected by curves. With additional control points, it is possible to model shapes of arbitrary complexity.

Interactive Design Environment

The present invention (in at least some implementations) includes an interactive

10   design environment for modeling semiconductors and other samples. Fundamentally, this is an environment that allows the types of models just described to be visually defined and evaluated. The following sections describe the components that combine to form the interactive design environment as well as their relationships to each other.

Figure 6 shows the main interface 600 for the visual design environment. Main

15   interface 600 includes a spectral fitting component 602, a film structure component 604, a layer property component 606, a global parameters component 608, and an interactive shape modeling component 610. As shown more clearly in Figure 7, spectral fitting component 602 compares the theoretically generated response from the model (such as the models described in Figure 5A through 5Q) to empirically obtained measurements. In

20   this sense, spectral fitting component 602 is the end result of the visual design environment providing the user with important feedback of the success or failure of the design process.

As shown in Figure 8, film structure component 604 includes a gross model definition. The gross model definition is a block like depiction of the layers that are

25   currently included in the sample being modeled. For the particular example of Figure 8, a five layer model is represented. This includes an upper layer (formed in photo-resist or PR), three intermediate layers (formed in SiARC, Poly and Thermal Oxide, respectively) and a substrate (formed in Crystalline Silicon).

A "Number of Films" control allows the user to increase or decrease the number

30   of layers included in the gross model definition. Increasing the number of layers causes the upper layer to be replicated. In this case, that would result in an extra photo-resist

layer being added to the top of the gross model definition. The type of material in each layer is interactively changeable (typically using a mouse activated popup menu). This allows the user to add layers, and then select the type of material used in the new layers. Decreasing the number of layers deletes the uppermost layer.

5   A "Number of Spacers" control allows the user to increase or decrease the number of spacers included in the gross model definition. Each spacer is created using a default material (typically replicating the material in the lowermost layer included in the line structure). The user may then interactively select an appropriate material as necessary (typically using a mouse activated popup menu).

10   A "Number of Trench Fills" control allows the user to increase or decrease the number of trench fills that are included in the gross model definition. Each trench fill is created using a default material (typically replicating the material in the lowermost layer included in the line structure). The user may then interactively select an appropriate material as necessary (typically using a mouse activated popup menu).

15   For the particular example of Figure 8, only the PR layer is included in the line profile of the sample being modeled. Visually, film structure component 602 distinguishes layers included in the line profile by making them appear as narrow rectangles sitting on top of the wider rectangles used to represent layers not included in the line profile. This gives the gross model definition a rough line profile that allows the

20 user to quickly deduce which layers are actually used to form the lines on the surface of a model. A "Number of Layers in Lines" control allows the user to increase or decrease the number of layers of this kind. In the case of Figure 8, incrementing the value of the control would cause the SiARC layer to be included in the line profile for the sample being modeled. Decreasing the number would remove the PR layer from the line profile,

25 leaving in this case, a model with no lines.

      Film structure component 602 also includes a series of buttons to control calculation. This includes a "Calc Once" button, a "Calc & Fit" button and a "Stop Fitting" button. The "Calc Once" causes the visual design environment to evaluate the current model and display the resulting spectra using the spectral fitting component 602.

30 The "Calc & Fit" button causes the visual design environment to initiate a regression-based analysis to minimize the differences between the spectra created by evaluating the

current model and empirically obtained spectra. The regression-based analysis iteratively changes model parameters to reduce the difference between evaluated and empirical results. As discussed below, the visual design environment allows the user to specify the parameters to be changed along with appropriate step sizes and other details. The "Stop
5   Fitting" button halts the regression process and displays the results of the last complete evaluation using the spectral fitting component 602.

Film structure component 602 includes a "Use Global Shape" option to enable or disable global definition (global shape definition is described above). An "Export Ini file" allows the user to specify and write a file containing a description of the current model.
10   This allows the current model to be saved and reloaded for later analysis. A "Reset" button undoes any modification made to the model, resetting it to an initial state. Typically, that state is defined as the initial model state as loaded from a file. A "Pick Data File" button allows the user to specify and load a file containing empirical measurements for the sample being modeled.

15   As shown in Figure 9, layer property component 606 includes a series of fields that describe a particular layer in the model being evaluated. For the specific example of Figure 9, the layer property component corresponds to the PR layer. This can be changed by selecting (typically by a mouse click) one of the other layers in the gross model definition within film structure component 602. The fields included in layer property
20   component 606 allow the user to specify the height of the corresponding layer using maximum, minimum and normal values. The user can also indicate whether variations in height should be used during regression analysis of the model. For the case where regression of this parameter is specified, the user can specify the number of steps to be used.

25   In a similar fashion, the fields included in layer property component 606 allow the user to specify the width of a layer using maximum, minimum and normal values. The user can also indicate whether variations in width should be used during regression analysis of the model. For the case where regression of this parameter is specified, the user can specify the number of steps to be used.

30   The "Add a Width" button allow the user to add additional control points to a layer. As an example, consider Figure 5A and 5B. The difference in these two figures is

the additional control point X_1 in Figure 5B. In the visual design environment, this can be accomplished by selecting upper layer 502a in the gross model definition and then activating the "Add a Width" button in the layer property component 606. Each added layer is given the same fields shown for existing layers allowing the user to select

5   maximum, minimum and normal widths as well as regression options. The "Delete a Width" button allows the user to remove control points from a layer.

Layer property component 606 also allows the user to specify the number of slices that will be used to evaluate each layer. Slicing is discussed in more detail below.

As shown in Figure 10, global parameters component 608 includes a series of

10   fields that are global to the model being evaluated (i.e., not specifically related to any particular layer or structure). These include fields allowing the user to specify the range of wavelengths used during regression ("From", "To" and "Step"). In the example shown in Figure 10, "Step" is set to five. This means that beginning from the 190 nm wavelength every 5th measured data point is used for the regression analysis. The choice

15   of the wavelength range is typically based on the usefulness of the data in terms of its information content, which for example may be influenced by the penetration depth of the incident light. Throughput considerations and the calculation speed also influence the choice of the wavelength discrimination

The "Max iterations" option controls the number of iterations the regression

20   algorithm should run. It is an integer value greater than zero. Higher numbers of iterations cause a longer computation time not necessarily yielding the global residual minimum. The choice of the iteration number must be made based on throughput considerations as well as the regression convergence performance after each sequence of the recipe. An iteration number between three and five is used for majority of the CD

25   optical models.

Another set of fields allows the user to specify the pitch (or line spacing) for the sample being modeled. These options take the form of normal, minimum and maximum values. The user can also specify whether line pitch is to be varied during regression. A final option allows the user to specify the type of measurement technology that will be

30   used. Currently, this list includes SE + DC (spectral ellipsometry with DC component), SE – DC (spectral ellipsometry without DC component), BB (broadband), SE + DC+ BB

(spectral ellipsometry with DC component and broadband) and SE – DC+ BB (spectral ellipsometry with broadband and without DC component). Additional information describing these parameters is found in US Patent Serial No. 6,278,519. The disclosure of that patent is included in this document by reference.

5   Global parameters component 608 also includes a "Show More Params" button. Activating this button invokes the additional parameters component shown in Figure 11. The additional parameters component includes the following fields:

"Measurement angle"	This parameter represents the azimuth angle, which is the deviation from the ideal ninety degree angle between the SE incident beam and the orientation of the grating lines.
"Mixing factor"	Fitting this parameter enables compensation for contributions made by the surrounding material.
"Side wall"	enables spacer considerations such as a coating native oxide layer on a silicon trench line.
"Eccentricity"	this parameter is related to BB spot anomaly correction.
"No. orders"	number of Fourier reconstruction orders. This number is material dependent. For example, for dielectric films "No. orders" may be nine or lower, whereas for semiconducting films the number might approach twenty or higher. The line spacing ratio can also influence the number of orders. Number of orders and calculation time are proportional.
"No. processors"	for systems that support multiple processors, this integer parameter can be chosen to be greater than one. Single processors systems require "No. processors" equal to one.
"Fitting option"	In addition to the more commonly exploited Levenberg-Marquard regression search engine, Simple Box, Simulated Annealing, Principal Axis and the DE Generic Algorithms may be selected.
"# of Phis (SE)"	An integer (> 0) that represents # of azimuthal angles used in numerical integration for SE.
"# of Thetas (SE)"	An integer (≥ 0) that represents # of incident angles used in

	integration for SE. # of Thetas = 0 activates the adaptive integration mode.
"# of Phis (BB)"	An integer in the range [0 10]. This parameter is related to the number of azimuthal angles used in integration for BB and is useful while using the conical model only.
"# of Thetas (BB)"	An integer in the range [-5, 10] which represents the number of incident angles used in integration for BB.
"Interpolation"	Cubic-spline is an example of one type of interpolation mode.
"Tolerance"	This option can be used together with the number of tries feature. It often results in significant timesavings during seed value determinations. The tolerance defines a lower residual limit for interruption of the calculations. In other words, the regression search terminates as soon as the residual value reaches the tolerance limit. Small tolerance values tend to increase the accuracy but also trade off with the calculation speed.
"Number of Tries"	This feature is often used during the initial sequence to determine correct seed values. The software divides the range into a number of sub intervals to more efficiently search for the optimum solution. The feature is time consuming, and once appropriate nominal values are determined, it is disabled in the final recipe. The Tolerance feature can be employed to achieve a faster nominal value search.
"Number of Slices"	This parameter identifies number of slices used for the sublayer. Assigning a negative sign to this number yields a smooth transition at the interface between the sublayer and the layer on top. It is realized by coupling the topmost shape control point of the sublayer to the lowest shape control point of the upper layer. The negative sign convention does not need to be used when the global shape option is employed.

As shown in Figure 11, the additional parameters component also includes a "Model option" parameter. This allows the user to select the underlying algorithm that will be used to perform model evaluations. The following algorithms may be specified:

"FTM-Simple"	layer-based RCWA Fourier expansion in the x-direction coupled with mode matching (matrix diagonalization) for vertical direction. FTM stands for Fast Transfer Matrix.
"FTM-Conical"	RCWA Fourier expansion in the x-direction coupled with mode matching for vertical direction. This algorithm is an improved RCWA approach using the so-called TM1 implementation. The model can handle overlays.
"G0-QMR"	(Quasi Minimal Residual Iterative Linear Solver): the model is a Green's function volume integral approach. It has proved to be a fast approach for low contrast materials.
"G1-QMR"	similar to the G0-QMR model. The Green's function is based on rectangular grating profiles. The model might be efficient for characterization of profiles that deviate little from straight ones.
"G-Born"	first order perturbation, simpler version of G1-QMR.
"GA-QMR"	generalized version of the G0-QMR model.
"FD-CON"	finite difference (vertical direction) conical version of the FD-CD model.
"FD-CD model"	non-conical finite difference model. It represents the fastest non-conical code. The model usually requires more slices than FTM-Simple model. It can switch to FTM-Simple for rectangular profiles.

5

The additional parameters component also includes a "Spline option" parameter. This parameter allows the user to control the way in which control points are spaced. The following values are supported:

0	Causes control points to be equally spaced.
[1, 10]	Causes control points to be more densely allocated near the boundaries with sigmoid-1.
[10, ∞)	Causes control points to be more densely allocated near the boundaries with sigmoid-2.
[-10, -1]	Causes control points to be more densely allocated at the top with sigmoid-2.
(-∞, -10)	Causes control points to be more densely allocated on the bottom with sigmoid-2.

5   The additional parameters component also includes a "Slicing option" parameter. This allows the user to specify the scheme that will be used to slice the model for evaluation. As shown in Figure 12A, the default slicing strategy divides the model into a series of equally sized slabs. Adaptive slicing, shown in Figure 12B optimizes slicing placement to reflect the geometry being modeled. In particular, adaptive slicing places

10   more slices near material boundaries (i.e., at layer tops and bottoms). Adaptive slicing also places more slices where sidewall geometry is complex or rapidly changing. Sigmoid slicing, shown in Figure 12C is a type of adaptive slicing that uses a sigmoid function to vary slice density to optimize layer interfaces and sidewall geometry.

The additional parameters component also includes a "Slice scale" parameter.

15   Slice scale provides a second mechanism for controlling the way layers within a model are sliced for evaluation. The following ranges are defined for slice scale:

$s \leq 0.5$	Number of slices (n_s) is controlled by the number of slices parameter.
$s > 0.5$ and slicing option set to "equally spaced" or "sigmoid."	n_s is defined as $\frac{1}{2}|\varepsilon| kt$ (where $k = 2\pi/\lambda$, t = height, and ε is the permittivity).

s > 0.5 and slicing option set to "adaptive."	$\left\|\dfrac{dw}{dh}\right\|\|e\|kt$	

As shown in Figure 13, interactive shape modeling component 610 includes a visual representation of the sample being modeled. For this particular example, interactive shape modeling component 610 displays five layers: an upper layer 1302,

5   intermediate layers 1302b through 1302d and a substrate 1302e. These correspond to the PR, SiARC, Poly, Thermal Oxide, and Crystalline Silicon layers described for the gross model definition of film structure component 602. In the visual design environment, the heights of the non-substrate layers 1302a through 1302d are defined by the position of respective control points Z_0 through Z_3. The width of upper layer 1302a (and all layers

10   included within the line profile) is defined by the control points X_0 and X_0'. The location of each control point is interactively movable, typically using a mouse or other pointing device. This allows the user to interactively change parameters such as layer thickness, line height and line width.

Interactive shape modeling component 610 works in concert with spectral fitting

15   component 602, film structure component 604, layer property component 606, and global parameters component 608. Changes made in any single component are reflected across the remaining components. As an example Figure 14A shows film structure component 604 after the "Number of Films" control has been increased from five to six. Within film structure component 604, this adds an additional layer to the gross model definition. As

20   shown in Figure 14B, this change is propagated to interactive shape modeling component 610 which now includes an additional layer and control point. As a second example, Figure 15A shows layer property component 606 after activation of the "Add a Width" button. Within layer property component 606, this adds an additional width with maximum, minimum, normal values as well as a regression option. As shown in Figure

25   15B, this change is propagated to interactive shape modeling component 610 which now includes an additional control point X_1. Interactively moving the control point X_1 as shown in Figure 15C, results in a corresponding change in the size of the second width of the layer property component 606 shown in Figure 15D.

Spectral fitting component 602 provides the user with visual feedback to guide the design process. As an example, Figure 16A shows a five layer sample displayed in the gross model definition of shows film structure component 604. Figure 16B shows the corresponding model displayed in interactive shape modeling component 610. Activating

5   the "Calc Once" button of film structure component 604 produces the spectra shown in spectral fitting component 602 of Figure 16C. At this point, the user can choose to interactively alter the model displayed in interactive shape modeling component 610 or take other steps to improve the goodness of fit. Figure 16D shows the case where the user has added an additional control point (using layer property component 606) and

10   interactively moved the new control point using (in interactive shape modeling component 610) to change the line profile of the sample being modeled. Hitting the "Calc Once" button a second time produces the spectra shown in spectral fitting component 602 of Figure 16E. By inspection, it is clear that there is now a much greater correspondence between expected and calculated spectra. This means that the change in line profile shape

15   was beneficial. Figures 16F and 16G show the result of the user activating the "Calc & Fit" button of film structure component 604. This has caused additional changes in the shape of the line profile being modeled and increased the goodness of fit between expected and calculated spectra.

In general, it is not possible to specify an exact sequence of steps used during a

20   typical use of the interactive environment. However, as shown in Figure 17, a user might begin such as session by loading an existing model typically located on disk or another secondary storage device. The existing model may be the end result of a previous use of the interactive environment, or may have been created in some other fashion, including manual specification. Loading the model causes all of the components of the visual

25   design environment to be updated. In particular, this means that the loaded model is shown, both in the gross model definition of film structure component 604, as well as in interactive shape modeling component 610.

Once loaded, the user will typically use the interactive environment to evaluate the model using the "Calc Once" or "Calc & Fit" buttons (represented by step 1704). This

30   causes the calculated spectral response information to be displayed along with the corresponding empirical response information in spectral fitting component 602. At this

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point, the user has a clear picture of how closely the model matches the corresponding empirical results. Typically, the user would then modify the model in some way. As represented by step 1706, this could include changes to global parameters through the use of the global parameters component 608. Alternately, film structure component 604 may

5   be used to alter the gross definition of the model (represented by step 1708). This could include, for example, adding or deleting layers, spacers or trench fills. Changes may also be made to individual layers using layer property component 606 (shown as step 1710). More intuitive are change made using interactive shape modeling component 610 (as shown in step 1712). To make these changes, the user drags control points within the

10   representation of the model in interactive shape modeling component 610. As the user makes these interactive changes, it is typically to use layer property component 606 to add or delete control points.

Once the user has made one or more model changes, it is typical to reevaluate the model using the "Calc Once" or "Calc & Fit" buttons (represented by step 1714). Once

15   again, the corresponding results are displayed along with the corresponding empirical response information in spectral fitting component 602. After the re-evaluation, the user can decide if the new calculated results are sufficiently close to the empirical data. Typically, the process of model modification followed by re-evaluation will be repeated for at least several iterations. In each case, the user is able to determine if each

20   incremental change is beneficial or harmful. This allows the user to proceed in an almost trial and error fashion where a series of educated guesses are used to refine the model until acceptable results are obtained. At that point, a typical use of the interactive environments ends with the user saving the modified model (see 1716).